



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:13 PM GMT

PDB ID : 4R5P
Title : Crystal structure of HIV-1 reverse transcriptase (RT) with DNA and a nucleoside triphosphate mimic alpha-carboxy nucleoside phosphonate inhibitor
Authors : Das, K.; Martinez, S.E.; Arnold, E.
Deposited on : 2014-08-21
Resolution : 2.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

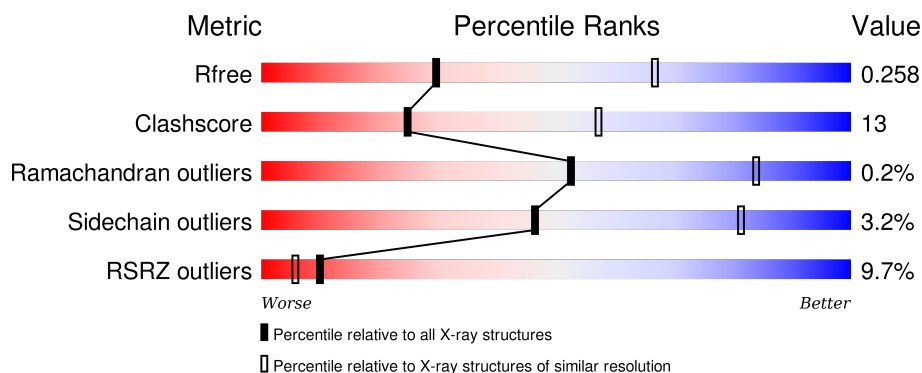
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	556	<div> <div>11%</div> <div>66%</div> <div>32%</div> <div>.</div> </div>
1	C	556	<div> <div>13%</div> <div>65%</div> <div>33%</div> <div>.</div> </div>
2	B	428	<div> <div>5%</div> <div>70%</div> <div>25%</div> <div>..</div> </div>
2	D	428	<div> <div>8%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
3	E	27	<div> <div>19%</div> <div>59%</div> <div>30%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	T	27	
4	F	21	
4	P	21	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	B	502	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17714 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HIV-1 reverse transcriptase, p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4511	2920	751	832	8			
1	C	554	Total	C	N	O	S	0	0	0
			4506	2917	750	831	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP P03366
A	0	VAL	-	EXPRESSION TAG	UNP P03366
A	258	CYS	GLN	ENGINEERED MUTATION	UNP P03366
A	280	SER	CYS	ENGINEERED MUTATION	UNP P03366
A	498	ASN	ASP	ENGINEERED MUTATION	UNP P03366
C	-1	MET	-	EXPRESSION TAG	UNP P03366
C	0	VAL	-	EXPRESSION TAG	UNP P03366
C	258	CYS	GLN	ENGINEERED MUTATION	UNP P03366
C	280	SER	CYS	ENGINEERED MUTATION	UNP P03366
C	498	ASN	ASP	ENGINEERED MUTATION	UNP P03366

- Molecule 2 is a protein called HIV-1 reverse transcriptase, p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3391	2204	562	619	6			
2	D	412	Total	C	N	O	S	0	0	0
			3393	2206	563	618	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED MUTATION	UNP P03366
D	280	SER	CYS	ENGINEERED MUTATION	UNP P03366

- Molecule 3 is a DNA chain called 5'-D(*TP*GP*GP*AP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	24	Total	C	N	O	P	0	0	0
			495	233	100	139	23			
3	E	24	Total	C	N	O	P	0	0	0
			495	233	100	139	23			

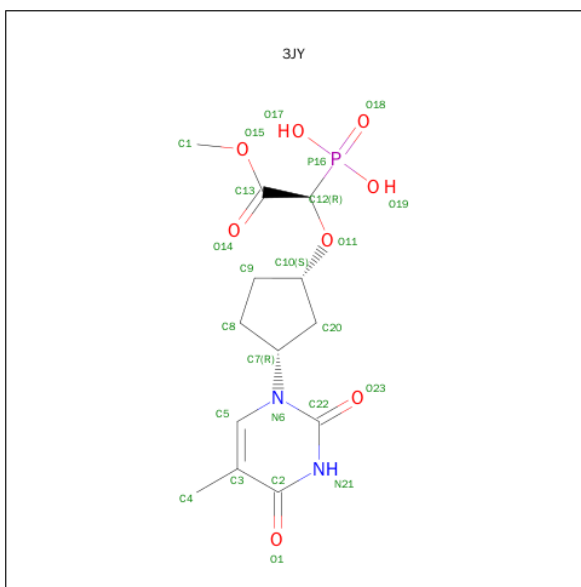
- Molecule 4 is a DNA chain called 5'-D(*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*G)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	P	20	Total	C	N	O	P	S	0	0	0
			407	195	72	120	19	1			
4	F	20	Total	C	N	O	P	S	0	0	0
			407	195	72	120	19	1			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

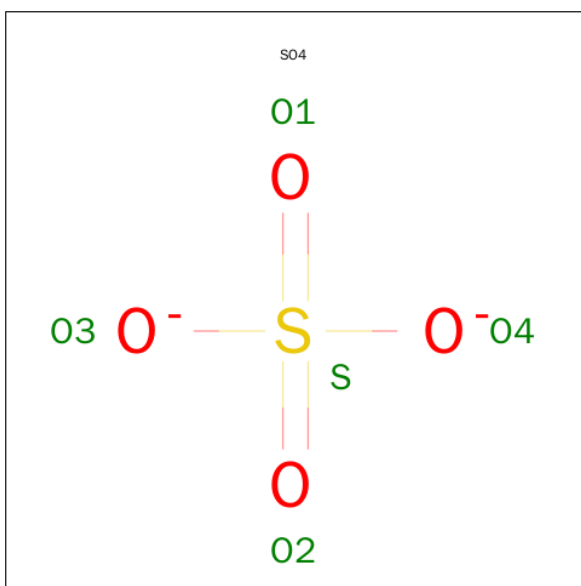
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	2	Total	Mg	0	0
			2	2		
5	D	1	Total	Mg	0	0
			1	1		
5	C	2	Total	Mg	0	0
			2	2		

- Molecule 6 is [(1R)-2-METHOXY-1-{[(1S,3R)-3-(5-METHYL-2,4-DIOXO-3,4-DIHYDRO-PYRIMIDIN-1(2H)-YL)CYCLOPENTYL]OXY}-2-OXOETHYL]PHOSPHONIC ACID (three-letter code: 3JY) (formula: C₁₃H₁₉N₂O₈P).



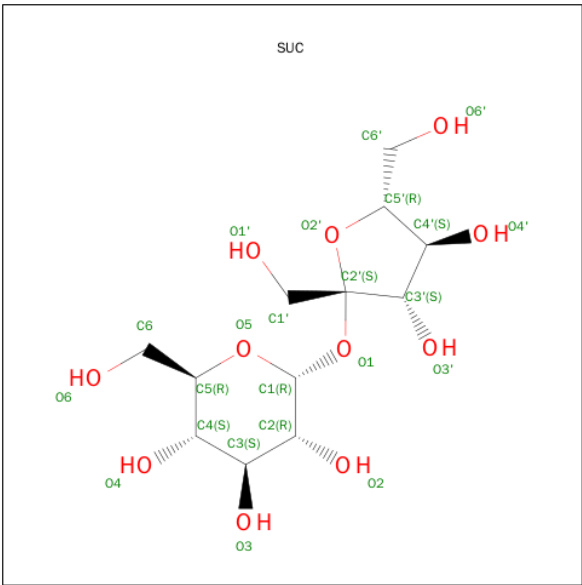
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			23	12	2	8	1		
6	C	1	Total	C	N	O	P	0	0
			23	12	2	8	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			23	12	11		
8	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	O	0	0
			1	1		
9	C	1	Total	O	0	0
			1	1		
9	B	2	Total	O	0	0
			2	2		
9	D	2	Total	O	0	0
			2	2		

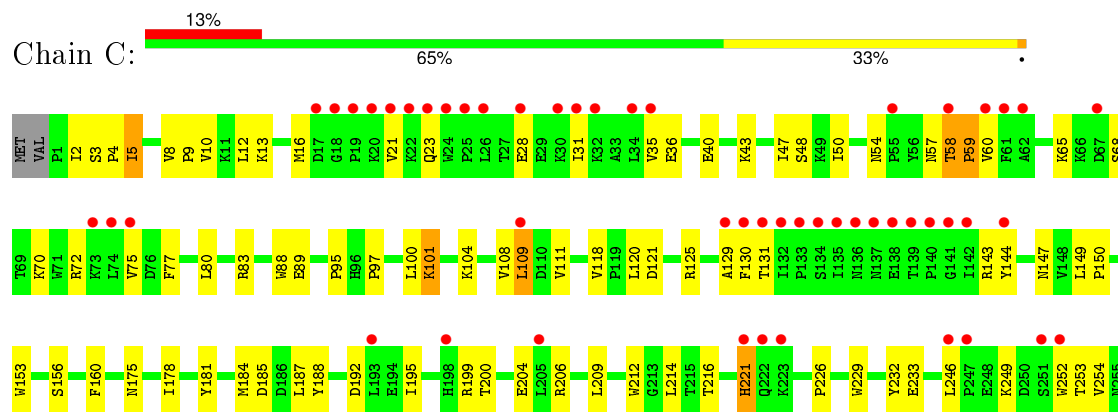
3 Residue-property plots

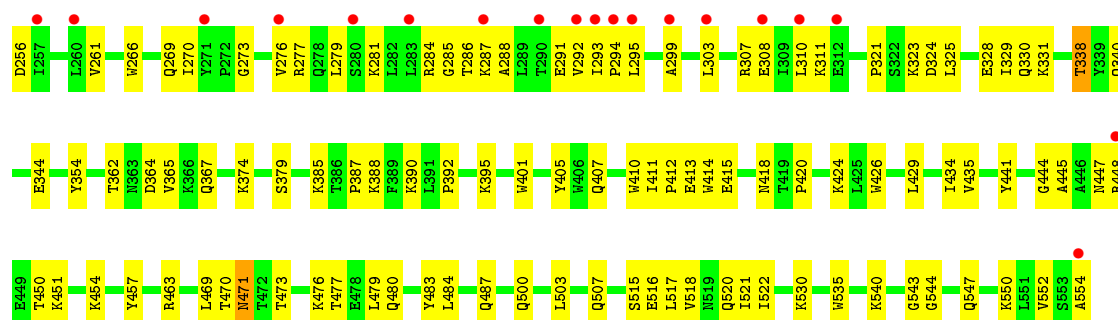
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: HIV-1 reverse transcriptase, p66 subunit

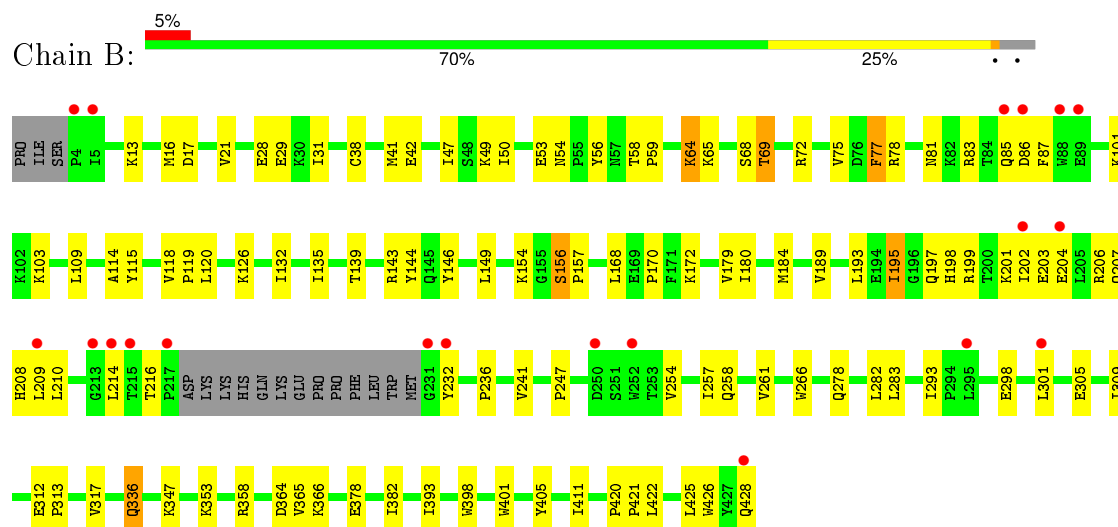


- Molecule 1: HIV-1 reverse transcriptase, p66 subunit

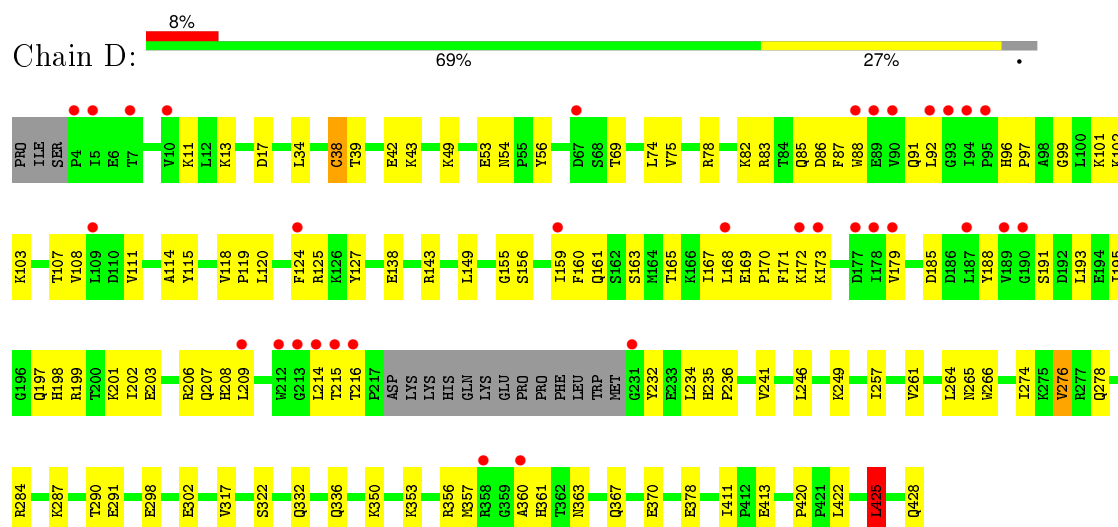




- Molecule 2: HIV-1 reverse transcriptase, p51 subunit

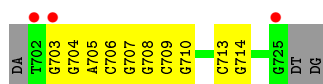


- Molecule 2: HIV-1 reverse transcriptase, p51 subunit



- Molecule 3: 5'-D(*TP*GP*GP*AP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*G)-3'





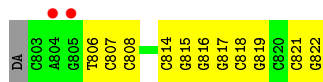
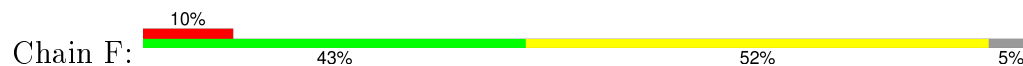
- Molecule 3: 5'-D(*TP*GP*GP*AP*CP*GP*GP*CP*GP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*G)-3'



- Molecule 4: 5'-D(*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*G)-3'



- Molecule 4: 5'-D(*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*G)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.91Å 133.53Å 139.22Å 90.00° 97.81° 90.00°	Depositor
Resolution (Å)	44.54 – 2.89 48.50 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.54-2.89) 99.1 (48.50-2.89)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.195 , 0.251 0.208 , 0.258	Depositor DCC
R_{free} test set	2152 reflections (3.08%)	DCC
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 72110 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17714	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MRG, MG, 3JY, SUC, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.60	0/4629	0.75	3/6290 (0.0%)
1	C	0.54	0/4624	0.69	1/6282 (0.0%)
2	B	0.63	0/3486	0.76	1/4735 (0.0%)
2	D	0.59	1/3489 (0.0%)	0.74	1/4740 (0.0%)
3	E	0.81	0/557	0.98	2/859 (0.2%)
3	T	0.85	0/557	0.96	0/859
4	F	0.93	0/424	1.07	1/649 (0.2%)
4	P	0.93	1/424 (0.2%)	1.03	0/649
All	All	0.63	2/18190 (0.0%)	0.77	9/25063 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	298	GLU	CG-CD	5.24	1.59	1.51
4	P	808	DC	C3'-O3'	-5.03	1.37	1.44

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	364	ASP	CB-CG-OD2	-6.29	112.63	118.30
1	A	325	LEU	CB-CG-CD1	-6.22	100.43	111.00
1	A	134	SER	CB-CA-C	5.54	120.63	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	703	DG	O4'-C4'-C3'	-5.25	102.40	104.50
1	A	551	LEU	CA-CB-CG	5.24	127.35	115.30
1	C	109	LEU	CA-CB-CG	5.15	127.15	115.30
3	E	703	DG	C4'-C3'-C2'	-5.15	98.47	103.10
4	F	821	DC	O4'-C4'-C3'	-5.10	102.46	104.50
2	D	425	LEU	N-CA-C	5.02	124.55	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	420	PRO	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4511	0	4570	126	0
1	C	4506	0	4568	124	0
2	B	3391	0	3425	89	0
2	D	3393	0	3426	83	0
3	E	495	0	268	7	0
3	T	495	0	268	11	0
4	F	407	0	229	11	0
4	P	407	0	229	9	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
6	A	23	0	14	4	0
6	C	23	0	14	2	0
7	C	5	0	0	0	0
8	B	23	0	22	1	0
8	D	23	0	22	5	0
9	A	1	0	0	0	0
9	B	2	0	0	0	0
9	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	2	0	0	1	0
All	All	17714	0	17055	442	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (442) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.56	0.85
2:B:209:LEU:HD22	2:B:214:LEU:HD23	1.57	0.85
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.60	0.84
2:D:209:LEU:HD22	2:D:214:LEU:HD23	1.58	0.84
2:D:115:TYR:HD2	2:D:156:SER:HB3	1.46	0.81
2:D:115:TYR:CD2	2:D:156:SER:HB3	2.17	0.79
1:C:125:ARG:HD3	1:C:147:ASN:HA	1.66	0.78
1:C:195:ILE:HD11	1:C:199:ARG:HH21	1.48	0.77
2:D:170:PRO:HB2	2:D:208:HIS:HE1	1.49	0.77
1:C:23:GLN:HG2	1:C:131:THR:HG23	1.67	0.76
2:B:317:VAL:HG12	2:B:347:LYS:HD3	1.69	0.75
2:B:193:LEU:HD13	2:B:197:GLN:HB3	1.68	0.75
1:C:444:GLY:C	1:C:552:VAL:HG11	2.06	0.75
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.69	0.74
2:B:195:ILE:HG22	2:B:199:ARG:HE	1.53	0.74
1:C:445:ALA:HB3	1:C:552:VAL:HG12	1.69	0.73
1:A:459:THR:HG22	1:A:461:LYS:H	1.54	0.72
1:A:56:TYR:O	1:A:143:ARG:NH2	2.21	0.71
2:B:47:ILE:HD12	2:B:144:TYR:CD2	2.26	0.71
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.74	0.70
4:F:807:DC:H2"	4:F:808:DC:H5"	1.73	0.70
2:D:287:LYS:NZ	2:D:291:GLU:OE2	2.25	0.69
2:D:170:PRO:HB2	2:D:208:HIS:CE1	2.27	0.69
4:P:816:DG:H2"	4:P:817:MRG:H8	1.75	0.69
1:C:285:GLY:HA2	3:E:714:DG:H5"	1.75	0.69
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.74	0.68
2:B:17:ASP:O	2:B:83:ARG:NH1	2.23	0.67
2:B:266:TRP:CD1	2:B:425:LEU:HD22	2.29	0.67
2:D:266:TRP:HD1	2:D:425:LEU:HD13	1.58	0.67
8:D:501:SUC:H1'2	8:D:501:SUC:O5	1.93	0.67
1:C:288:ALA:HB3	1:C:291:GLU:HB2	1.77	0.67
1:C:354:TYR:HD1	1:C:374:LYS:HD3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:284:ARG:HG2	2:D:284:ARG:HH11	1.59	0.67
1:C:454:LYS:HE3	1:C:554:ALA:O	1.94	0.67
2:D:199:ARG:HA	2:D:202:ILE:HD12	1.76	0.66
1:A:308:GLU:HA	1:A:311:LYS:HG3	1.76	0.66
2:D:13:LYS:NZ	2:D:85:GLN:OE1	2.28	0.66
1:C:448:ARG:O	1:C:451:LYS:NZ	2.29	0.66
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.31	0.65
1:C:445:ALA:N	1:C:552:VAL:HG11	2.12	0.65
2:B:422:LEU:H	2:B:422:LEU:HD23	1.62	0.65
6:A:602:3JY:H11	6:A:602:3JY:H6	1.77	0.65
1:C:445:ALA:CB	1:C:552:VAL:HG12	2.27	0.64
2:D:357:MET:HB3	2:D:370:GLU:OE1	1.97	0.64
2:D:168:LEU:HB3	2:D:172:LYS:HE3	1.79	0.64
1:A:543:GLY:HA2	2:B:283:LEU:O	1.96	0.64
1:C:253:THR:HG22	1:C:292:VAL:HG12	1.79	0.64
1:C:434:ILE:HD13	1:C:530:LYS:HB3	1.78	0.64
1:C:535:TRP:CD2	2:D:422:LEU:HD21	2.33	0.64
1:A:24:TRP:CE3	1:A:25:PRO:HD2	2.34	0.63
2:D:111:VAL:HG23	2:D:115:TYR:HE1	1.62	0.63
2:D:206:ARG:NH1	2:D:216:THR:O	2.32	0.63
1:A:175:ASN:HB3	1:A:178:ILE:HG12	1.79	0.63
2:D:17:ASP:O	2:D:83:ARG:NH1	2.29	0.63
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.79	0.63
2:D:86:ASP:OD1	2:D:87:PHE:N	2.32	0.63
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.81	0.63
1:C:445:ALA:N	1:C:552:VAL:CG1	2.62	0.62
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.81	0.62
1:C:293:ILE:HG13	1:C:294:PRO:HD2	1.80	0.62
1:A:76:ASP:OD2	1:A:78:ARG:NH2	2.26	0.62
1:C:246:LEU:HD11	1:C:310:LEU:HD22	1.81	0.62
2:D:87:PHE:HZ	2:D:159:ILE:HG13	1.63	0.62
3:T:703:DG:C2	3:T:704:DG:H1'	2.34	0.62
2:B:109:LEU:HD22	2:B:216:THR:HG21	1.82	0.62
4:F:807:DC:H2''	4:F:808:DC:C5'	2.29	0.61
2:B:197:GLN:O	2:B:201:LYS:HG2	2.01	0.61
1:A:459:THR:CG2	1:A:461:LYS:H	2.13	0.61
2:B:257:ILE:O	2:B:261:VAL:HG23	2.00	0.61
1:C:362:THR:HG21	1:C:367:GLN:HE21	1.63	0.61
2:B:198:HIS:CD2	2:B:202:ILE:HD11	2.35	0.61
1:A:452:LEU:HD23	1:A:470:THR:HA	1.82	0.61
2:D:356:ARG:HD3	2:D:361:HIS:HE1	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:VAL:HG11	1:A:73:LYS:HE2	1.82	0.61
2:D:120:LEU:HD11	2:D:124:PHE:HD2	1.66	0.61
1:C:21:VAL:HG23	1:C:59:PRO:HD3	1.82	0.61
2:D:114:ALA:HB2	2:D:214:LEU:HD22	1.82	0.60
2:D:115:TYR:O	2:D:149:LEU:HB2	2.01	0.60
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.36	0.60
1:C:470:THR:HG22	1:C:471:ASN:HB2	1.81	0.60
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.35	0.60
1:A:438:GLU:OE2	1:A:459:THR:HG21	2.01	0.60
2:D:266:TRP:CD1	2:D:425:LEU:HD13	2.36	0.60
1:C:500:GLN:HG2	2:D:422:LEU:HD22	1.83	0.60
2:B:65:LYS:HB3	2:B:232:TYR:OH	2.00	0.60
1:A:293:ILE:HG13	1:A:294:PRO:HD2	1.84	0.60
1:C:516:GLU:O	1:C:520:GLN:HG3	2.01	0.60
8:B:501:SUC:H1'2	8:B:501:SUC:O5	2.02	0.60
1:C:331:LYS:HE3	1:C:364:ASP:OD2	2.02	0.59
1:C:261:VAL:HG13	1:C:276:VAL:HG11	1.83	0.59
2:D:261:VAL:HG13	2:D:276:VAL:HG11	1.84	0.59
1:C:535:TRP:CE2	2:D:422:LEU:HD21	2.38	0.58
1:C:308:GLU:HA	1:C:311:LYS:HG3	1.85	0.58
1:A:500:GLN:HG2	2:B:422:LEU:HD13	1.84	0.58
4:F:818:DC:H2'	4:F:819:DG:H8	1.67	0.58
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.86	0.57
1:C:518:VAL:O	1:C:522:ILE:HG13	2.04	0.57
1:A:250:ASP:OD1	1:A:250:ASP:N	2.36	0.57
1:C:473:THR:O	1:C:477:THR:HG23	2.05	0.57
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.20	0.57
1:C:175:ASN:HB3	1:C:178:ILE:HD13	1.85	0.57
2:B:336:GLN:HG2	2:B:353:LYS:HD2	1.86	0.57
2:B:195:ILE:O	2:B:199:ARG:HG3	2.04	0.56
1:A:253:THR:HA	1:A:292:VAL:HA	1.87	0.56
1:A:60:VAL:HG22	1:A:75:VAL:HG13	1.88	0.56
1:A:281:LYS:HG3	1:A:284:ARG:NH1	2.20	0.56
3:T:713:DC:H2'	3:T:714:DG:C8	2.40	0.56
1:A:107:THR:OG1	1:A:198:HIS:NE2	2.32	0.56
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.86	0.56
2:B:154:LYS:HG2	2:B:184:MET:SD	2.45	0.56
1:A:284:ARG:HG3	3:T:713:DC:H5"	1.87	0.56
1:A:273:GLY:HA2	1:A:338:THR:HG21	1.87	0.56
2:D:85:GLN:HA	2:D:88:TRP:CE2	2.41	0.56
2:B:56:TYR:HE2	2:B:126:LYS:HE2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:PRO:HG2	1:A:119:PRO:HD3	1.86	0.55
1:A:125:ARG:HD3	1:A:147:ASN:HD22	1.72	0.55
4:P:807:DC:H2''	4:P:808:DC:C5'	2.37	0.55
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.87	0.55
1:A:20:LYS:HA	1:A:57:ASN:H	1.71	0.55
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.88	0.55
4:F:818:DC:H2'	4:F:819:DG:C8	2.42	0.55
2:B:101:LYS:O	2:B:236:PRO:HB2	2.06	0.55
1:C:118:VAL:HB	1:C:149:LEU:HD12	1.89	0.54
2:D:168:LEU:O	2:D:171:PHE:N	2.40	0.54
2:B:86:ASP:CG	2:B:87:PHE:H	2.09	0.54
1:A:448:ARG:O	1:A:451:LYS:NZ	2.41	0.54
2:B:115:TYR:CD2	2:B:156:SER:HB3	2.42	0.54
1:C:72:ARG:NH2	6:C:602:3JY:O19	2.41	0.54
1:C:303:LEU:O	1:C:307:ARG:HG3	2.08	0.54
1:C:226:PRO:HB2	1:C:233:GLU:HB3	1.88	0.54
1:A:115:TYR:HD2	1:A:151:GLN:HG2	1.73	0.54
2:B:120:LEU:HD12	2:B:149:LEU:HD23	1.89	0.54
1:C:101:LYS:HE2	1:C:321:PRO:HG3	1.89	0.54
1:C:100:LEU:HD11	1:C:229:TRP:CZ3	2.43	0.54
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.89	0.54
2:B:266:TRP:NE1	2:B:425:LEU:HD22	2.22	0.54
2:D:78:ARG:HD3	2:D:411:ILE:O	2.08	0.54
2:D:363:ASN:O	2:D:367:GLN:HG3	2.08	0.53
3:E:713:DC:H2'	3:E:714:DG:C8	2.44	0.53
1:C:457:TYR:HE1	1:C:463:ARG:HG2	1.74	0.53
1:A:418:ASN:O	1:A:420:PRO:HD3	2.09	0.53
2:D:99:GLY:HA2	2:D:102:LYS:HD2	1.90	0.53
1:C:329:ILE:O	1:C:392:PRO:HD3	2.09	0.53
1:A:548:VAL:O	1:A:552:VAL:HG22	2.08	0.53
1:A:265:ASN:OD1	1:A:353:LYS:NZ	2.24	0.53
1:C:118:VAL:HG21	1:C:160:PHE:HD1	1.74	0.53
2:D:163:SER:O	2:D:167:ILE:HG13	2.09	0.53
3:T:703:DG:C5	3:T:704:DG:H8	2.27	0.53
2:B:64:LYS:NZ	2:B:69:THR:HA	2.24	0.53
2:D:78:ARG:O	2:D:82:LYS:HG3	2.09	0.52
4:F:814:DC:H2''	4:F:815:DG:C8	2.44	0.52
1:C:325:LEU:HB2	1:C:385:LYS:HE2	1.91	0.52
1:C:153:TRP:HB3	1:C:156:SER:OG	2.09	0.52
1:C:284:ARG:HB3	3:E:714:DG:OP1	2.10	0.52
2:B:86:ASP:CG	2:B:87:PHE:N	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ASP:O	2:B:83:ARG:HD3	2.10	0.52
1:C:287:LYS:HG3	1:C:288:ALA:H	1.74	0.52
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.44	0.52
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.92	0.52
1:C:21:VAL:CG2	1:C:59:PRO:HD3	2.40	0.52
1:C:209:LEU:O	1:C:214:LEU:HB2	2.10	0.52
2:D:357:MET:O	2:D:360:ALA:HB2	2.10	0.52
2:D:235:HIS:N	2:D:236:PRO:HD3	2.23	0.52
1:C:473:THR:OG1	1:C:476:LYS:HG3	2.09	0.51
4:P:807:DC:H2''	4:P:808:DC:H5''	1.91	0.51
1:C:435:VAL:HG22	2:D:290:THR:HG21	1.92	0.51
1:A:5:ILE:HG22	1:A:212:TRP:HD1	1.76	0.51
1:C:483:TYR:O	1:C:487:GLN:HG3	2.11	0.51
1:C:111:VAL:HB	1:C:185:ASP:HB2	1.92	0.51
3:E:713:DC:H2''	3:E:714:DG:H5'	1.93	0.51
2:B:16:MET:HG2	2:B:83:ARG:HG2	1.92	0.51
1:C:445:ALA:HB3	1:C:552:VAL:CG1	2.39	0.51
1:C:424:LYS:HE2	1:C:426:TRP:CE3	2.45	0.51
2:D:107:THR:HG23	2:D:232:TYR:HB3	1.92	0.51
1:C:445:ALA:CB	1:C:552:VAL:CG1	2.89	0.51
1:A:206:ARG:NH2	1:A:216:THR:O	2.44	0.51
1:A:209:LEU:O	1:A:214:LEU:HB2	2.11	0.50
1:C:12:LEU:HB3	1:C:83:ARG:O	2.11	0.50
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.92	0.50
2:D:114:ALA:HB1	2:D:160:PHE:CZ	2.47	0.50
1:C:435:VAL:HA	2:D:290:THR:HG21	1.94	0.50
3:E:716:DA:H2''	3:E:717:DC:OP2	2.11	0.50
2:B:114:ALA:N	2:B:214:LEU:HD13	2.27	0.50
2:B:149:LEU:HB3	2:B:156:SER:OG	2.11	0.50
2:B:207:GLN:HA	2:B:210:LEU:HD12	1.93	0.50
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.94	0.50
2:D:197:GLN:O	2:D:201:LYS:HG2	2.12	0.50
1:C:273:GLY:HA2	1:C:338:THR:HG21	1.93	0.50
2:B:69:THR:O	2:B:69:THR:HG23	2.12	0.50
1:A:167:ILE:O	1:A:170:PRO:HD2	2.11	0.50
2:D:332:GLN:HB2	2:D:336:GLN:HB3	1.93	0.49
1:A:221:HIS:ND1	1:A:221:HIS:N	2.60	0.49
2:B:198:HIS:O	2:B:202:ILE:HG13	2.12	0.49
1:C:89:GLU:HG3	3:E:708:DG:OP1	2.12	0.49
1:C:543:GLY:O	1:C:547:GLN:NE2	2.45	0.49
1:A:328:GLU:HG2	1:A:330:GLN:NE2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:TYR:O	2:B:149:LEU:HB2	2.12	0.49
1:C:254:VAL:HG21	1:C:286:THR:HG21	1.93	0.49
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.52	0.49
1:A:128:THR:HG21	1:A:146:TYR:HB2	1.94	0.49
1:C:390:LYS:HG2	1:C:415:GLU:HG2	1.94	0.49
1:A:77:PHE:O	1:A:80:LEU:N	2.44	0.49
2:B:50:ILE:HD11	2:B:143:ARG:HH21	1.76	0.49
1:A:184:MET:HG2	4:P:822:DG:H2''	1.93	0.49
1:C:150:PRO:HG2	1:C:153:TRP:HB2	1.94	0.49
1:A:56:TYR:HB2	1:A:129:ALA:HB3	1.94	0.49
1:A:38:CYS:SG	1:A:132:ILE:HD13	2.52	0.49
2:D:17:ASP:O	2:D:83:ARG:HD3	2.13	0.49
1:A:332:GLN:OE1	1:A:338:THR:HG23	2.12	0.49
1:A:500:GLN:CG	2:B:422:LEU:HD13	2.43	0.48
2:B:298:GLU:CD	2:B:298:GLU:H	2.16	0.48
2:B:157:PRO:HG3	2:B:184:MET:HA	1.95	0.48
2:B:247:PRO:HA	2:B:428:GLN:HE22	1.78	0.48
2:B:203:GLU:O	2:B:207:GLN:HG2	2.14	0.48
2:B:254:VAL:O	2:B:258:GLN:HG3	2.14	0.48
1:C:184:MET:HG2	4:F:822:DG:H2''	1.96	0.48
2:D:118:VAL:HG12	2:D:119:PRO:O	2.13	0.48
1:C:418:ASN:O	1:C:420:PRO:HD3	2.14	0.48
1:C:441:TYR:CG	1:C:544:GLY:HA3	2.49	0.48
1:A:230:MET:HE3	4:P:821:DC:H4'	1.94	0.48
1:A:457:TYR:HE1	1:A:463:ARG:HG2	1.78	0.48
1:C:388:LYS:HE2	1:C:413:GLU:OE2	2.14	0.48
1:C:503:LEU:HD11	1:C:507:GLN:HE21	1.77	0.48
2:B:69:THR:CG2	2:B:69:THR:O	2.61	0.48
2:B:168:LEU:HB3	2:B:172:LYS:HE3	1.96	0.47
1:C:36:GLU:O	1:C:40:GLU:HG2	2.14	0.47
1:A:58:THR:HG22	1:A:129:ALA:O	2.14	0.47
4:F:817:MRG:H2'	4:F:818:DC:C6	2.49	0.47
1:A:427:TYR:O	1:A:509:GLN:NE2	2.47	0.47
2:D:161:GLN:O	2:D:165:THR:HG22	2.14	0.47
2:B:77:PHE:O	2:B:81:ASN:ND2	2.47	0.47
1:C:13:LYS:O	1:C:16:MET:HB2	2.14	0.47
1:C:50:ILE:HG12	1:C:143:ARG:O	2.14	0.47
1:C:104:LYS:HB3	1:C:192:ASP:HA	1.95	0.47
2:D:191:SER:OG	2:D:198:HIS:ND1	2.26	0.47
1:C:125:ARG:HH11	1:C:147:ASN:HB3	1.80	0.47
2:B:109:LEU:HD22	2:B:216:THR:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:ARG:HB2	1:C:463:ARG:HE	1.44	0.47
1:A:340:GLN:HG3	1:A:351:THR:HG22	1.95	0.47
1:A:122:GLU:OE2	1:A:125:ARG:NH1	2.48	0.47
1:C:266:TRP:O	1:C:269:GLN:HG2	2.15	0.47
1:A:28:GLU:HB2	1:A:135:ILE:CD1	2.44	0.47
2:B:78:ARG:HD3	2:B:411:ILE:O	2.15	0.47
2:B:199:ARG:HA	2:B:202:ILE:HD12	1.97	0.47
2:D:82:LYS:HD3	2:D:413:GLU:OE1	2.14	0.47
8:D:501:SUC:O3'	8:D:501:SUC:H1	2.14	0.47
1:A:121:ASP:O	1:A:125:ARG:HG3	2.15	0.47
4:P:807:DC:H2''	4:P:808:DC:O5'	2.15	0.47
4:F:815:DG:H2''	4:F:816:DG:OP2	2.13	0.47
1:A:28:GLU:HB2	1:A:135:ILE:HD12	1.96	0.47
2:D:101:LYS:NZ	9:D:602:HOH:O	2.47	0.47
1:C:120:LEU:HD12	1:C:121:ASP:H	1.80	0.47
8:D:501:SUC:H1'2	8:D:501:SUC:C5	2.44	0.47
1:A:88:TRP:CD1	2:B:143:ARG:NH1	2.82	0.47
1:A:78:ARG:HH21	3:T:705:DA:H5'	1.80	0.46
2:D:257:ILE:O	2:D:261:VAL:HG23	2.15	0.46
3:T:709:DC:H2'	3:T:710:DG:C8	2.50	0.46
1:C:405:TYR:CE2	1:C:407:GLN:HB2	2.51	0.46
6:A:602:3JY:O14	6:A:602:3JY:O17	2.29	0.46
1:A:406:TRP:CD1	1:A:407:GLN:HG3	2.51	0.46
1:A:406:TRP:CH2	1:A:508:ALA:HB2	2.49	0.46
1:A:36:GLU:O	1:A:40:GLU:HG3	2.15	0.46
1:C:444:GLY:CA	1:C:552:VAL:HG11	2.46	0.46
1:A:401:TRP:HB2	1:A:425:LEU:HD11	1.97	0.46
1:A:145:GLN:O	1:A:145:GLN:HG3	2.16	0.46
2:D:336:GLN:OE1	2:D:353:LYS:HE3	2.16	0.46
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.51	0.46
1:C:65:LYS:HD2	1:C:70:LYS:HG3	1.98	0.46
2:D:360:ALA:HA	2:D:367:GLN:NE2	2.31	0.46
4:F:814:DC:H2''	4:F:815:DG:H8	1.80	0.46
1:A:363:ASN:O	1:A:367:GLN:HG3	2.16	0.46
1:A:21:VAL:N	1:A:57:ASN:O	2.36	0.46
3:T:713:DC:H2''	3:T:714:DG:H5'	1.98	0.46
1:C:365:VAL:HG11	1:C:401:TRP:CD1	2.51	0.46
1:A:21:VAL:HG23	1:A:58:THR:HA	1.99	0.45
1:A:325:LEU:HD12	1:A:385:LYS:HE2	1.97	0.45
1:C:281:LYS:HA	1:C:284:ARG:HG3	1.98	0.45
2:D:42:GLU:OE2	2:D:49:LYS:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ILE:O	1:A:341:ILE:HA	2.16	0.45
2:B:198:HIS:NE2	2:B:202:ILE:HD11	2.31	0.45
1:A:132:ILE:HD11	1:A:144:TYR:CD2	2.52	0.45
1:C:54:ASN:HB3	1:C:143:ARG:HH12	1.82	0.45
2:D:103:LYS:HD2	2:D:191:SER:C	2.37	0.45
2:D:191:SER:HB2	2:D:193:LEU:HG	1.98	0.45
2:D:203:GLU:O	2:D:207:GLN:HG2	2.17	0.45
1:A:459:THR:HG22	1:A:461:LYS:N	2.26	0.45
2:B:31:ILE:HD12	2:B:135:ILE:HG12	1.99	0.45
2:B:68:SER:O	2:B:69:THR:HB	2.15	0.45
2:D:108:VAL:HG22	2:D:188:TYR:CD1	2.52	0.45
1:A:266:TRP:CD2	4:P:820:DC:H4'	2.52	0.45
1:C:60:VAL:HG23	1:C:75:VAL:HG22	1.97	0.45
1:A:78:ARG:NH2	3:T:705:DA:H5'	2.32	0.45
1:A:305:GLU:O	1:A:309:ILE:HG13	2.17	0.45
1:A:202:ILE:HD13	1:A:202:ILE:HA	1.73	0.45
1:C:328:GLU:HG3	1:C:390:LYS:HB2	1.98	0.45
1:C:447:ASN:HB3	1:C:450:THR:HB	1.99	0.45
2:B:56:TYR:CE2	2:B:126:LYS:HE2	2.51	0.45
1:C:323:LYS:HE2	1:C:344:GLU:OE2	2.17	0.45
1:C:379:SER:CB	1:C:387:PRO:HD3	2.46	0.45
1:A:365:VAL:HG11	1:A:401:TRP:CD1	2.52	0.44
2:B:28:GLU:HA	2:B:135:ILE:HD11	1.99	0.44
1:C:57:ASN:OD1	1:C:131:THR:HG22	2.17	0.44
1:A:78:ARG:HE	1:A:78:ARG:HB2	1.58	0.44
2:B:232:TYR:N	2:B:232:TYR:CD1	2.85	0.44
1:A:118:VAL:HA	1:A:119:PRO:HD2	1.88	0.44
1:A:115:TYR:CD2	1:A:151:GLN:HG2	2.53	0.44
1:C:48:SER:O	1:C:144:TYR:HA	2.17	0.44
1:C:279:LEU:HD23	1:C:299:ALA:HB1	2.00	0.44
1:A:402:TRP:HB2	1:A:409:THR:HG23	2.00	0.44
3:E:722:DA:H2''	3:E:723:DC:C6	2.53	0.44
1:A:379:SER:CB	1:A:387:PRO:HD3	2.46	0.44
1:A:320:ASP:OD1	1:A:322:SER:OG	2.25	0.44
2:D:13:LYS:HD3	2:D:86:ASP:H	1.82	0.44
2:B:42:GLU:OE2	2:B:49:LYS:HG3	2.18	0.44
2:D:87:PHE:CZ	2:D:159:ILE:HG13	2.49	0.43
1:C:365:VAL:HG11	1:C:401:TRP:CG	2.53	0.43
2:D:56:TYR:CE2	2:D:127:TYR:CE1	3.06	0.43
1:C:540:LYS:HE3	2:D:265:ASN:OD1	2.17	0.43
1:A:84:THR:HG22	1:A:85:GLN:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:350:LYS:HE2	2:D:378:GLU:OE1	2.18	0.43
2:B:13:LYS:NZ	2:B:85:GLN:HB3	2.33	0.43
1:A:132:ILE:O	1:A:141:GLY:HA3	2.18	0.43
1:A:473:THR:HG23	1:A:476:LYS:HG3	1.99	0.43
1:C:479:LEU:HD23	1:C:479:LEU:HA	1.68	0.43
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.54	0.43
1:C:97:PRO:HD3	1:C:232:TYR:CE2	2.53	0.43
1:A:329:ILE:HD11	1:A:375:ILE:HD12	2.00	0.43
2:D:249:LYS:HB3	2:D:249:LYS:HE3	1.64	0.43
1:C:72:ARG:NH2	6:C:602:3JY:H3	2.34	0.43
2:B:13:LYS:CE	2:B:85:GLN:HB3	2.49	0.43
1:C:8:VAL:HA	1:C:9:PRO:HD2	1.76	0.43
1:A:50:ILE:HG12	1:A:143:ARG:O	2.19	0.43
1:A:169:GLU:N	1:A:170:PRO:HD2	2.34	0.43
1:A:10:VAL:HG11	1:A:153:TRP:CH2	2.53	0.43
1:C:129:ALA:HA	1:C:144:TYR:O	2.18	0.43
2:B:53:GLU:HG2	2:B:54:ASN:N	2.33	0.43
1:C:249:LYS:HG2	1:C:256:ASP:OD2	2.18	0.43
1:C:31:ILE:O	1:C:35:VAL:HG23	2.19	0.43
1:A:70:LYS:HA	1:A:70:LYS:HD3	1.75	0.43
6:A:602:3JY:H6	6:A:602:3JY:H3	1.74	0.43
1:A:376:THR:HG23	1:A:386:THR:HG23	2.01	0.43
1:C:429:LEU:HD23	1:C:429:LEU:N	2.32	0.43
1:A:163:SER:O	1:A:167:ILE:HG13	2.18	0.43
1:C:5:ILE:CG2	1:C:212:TRP:HD1	2.31	0.43
1:C:206:ARG:HG2	1:C:216:THR:OG1	2.19	0.43
2:D:43:LYS:NZ	2:D:43:LYS:HB2	2.34	0.43
2:B:204:GLU:O	2:B:208:HIS:HB2	2.19	0.43
3:T:709:DC:H2'	3:T:710:DG:H8	1.82	0.43
1:A:91:GLN:O	3:T:708:DG:H4'	2.18	0.43
1:A:131:THR:HB	1:A:143:ARG:HG2	2.00	0.42
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.54	0.42
2:D:87:PHE:HE2	2:D:155:GLY:HA2	1.85	0.42
1:C:484:LEU:HD23	1:C:487:GLN:HE21	1.84	0.42
1:A:226:PRO:HB3	1:A:235:HIS:NE2	2.34	0.42
1:C:441:TYR:CD2	1:C:544:GLY:HA3	2.54	0.42
1:C:410:TRP:CH2	1:C:412:PRO:HA	2.55	0.42
2:D:69:THR:O	2:D:69:THR:HG22	2.19	0.42
2:D:214:LEU:HD12	2:D:215:THR:N	2.34	0.42
1:C:411:ILE:HG22	1:C:412:PRO:O	2.19	0.42
1:C:469:LEU:HD11	1:C:480:GLN:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:GLU:O	2:B:309:ILE:HG13	2.19	0.42
1:C:181:TYR:CD1	2:D:138:GLU:HG3	2.55	0.42
1:C:5:ILE:HG22	1:C:212:TRP:CD1	2.55	0.42
2:B:358:ARG:HG3	2:B:366:LYS:HD3	2.01	0.42
2:D:169:GLU:O	2:D:173:LYS:HG2	2.20	0.42
2:D:53:GLU:HG2	2:D:54:ASN:N	2.35	0.42
2:B:393:ILE:HG21	2:B:398:TRP:HB2	2.02	0.42
2:B:41:MET:HE2	2:B:47:ILE:HG12	2.00	0.42
2:B:301:LEU:HD23	2:B:301:LEU:HA	1.73	0.42
1:A:441:TYR:N	1:A:441:TYR:CD1	2.87	0.42
1:A:334:GLN:O	1:A:336:GLN:HG3	2.19	0.42
1:C:434:ILE:CD1	1:C:530:LYS:HB3	2.48	0.42
2:B:425:LEU:HD23	2:B:426:TRP:CE2	2.55	0.42
1:C:8:VAL:O	1:C:10:VAL:HG23	2.19	0.42
1:A:362:THR:OG1	1:A:363:ASN:N	2.52	0.42
1:C:517:LEU:O	1:C:521:ILE:HG13	2.20	0.42
1:A:115:TYR:O	1:A:149:LEU:HB2	2.20	0.42
2:D:160:PHE:O	2:D:160:PHE:CD1	2.73	0.41
2:B:47:ILE:HG22	2:B:146:TYR:HA	2.02	0.41
1:A:3:SER:HA	1:A:4:PRO:HD3	1.96	0.41
1:A:125:ARG:HD3	1:A:147:ASN:HA	2.02	0.41
1:C:68:SER:OG	1:C:70:LYS:HG2	2.20	0.41
3:T:706:DC:H2'	3:T:707:DG:C8	2.55	0.41
1:C:395:LYS:HD2	1:C:414:TRP:CH2	2.55	0.41
1:A:238:LYS:HB2	1:A:315:HIS:ND1	2.35	0.41
8:D:501:SUC:HO6'	8:D:501:SUC:C2'	2.32	0.41
2:B:282:LEU:HB3	2:B:293:ILE:HG21	2.01	0.41
1:A:516:GLU:O	1:A:520:GLN:HG3	2.20	0.41
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.80	0.41
1:C:200:THR:O	1:C:204:GLU:HG3	2.20	0.41
4:F:807:DC:H2''	4:F:808:DC:O5'	2.19	0.41
4:P:807:DC:H4'	4:P:808:DC:OP1	2.21	0.41
1:A:329:ILE:O	1:A:392:PRO:HD3	2.20	0.41
1:C:77:PHE:O	1:C:80:LEU:N	2.54	0.41
1:C:43:LYS:HB2	1:C:43:LYS:HE3	1.62	0.41
1:A:135:ILE:HG13	1:A:136:ASN:OD1	2.20	0.41
2:B:58:THR:CG2	2:B:75:VAL:HG12	2.51	0.41
2:D:167:ILE:O	2:D:208:HIS:NE2	2.52	0.41
2:D:185:ASP:OD1	2:D:185:ASP:N	2.54	0.41
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.54	0.41
2:D:120:LEU:HD23	2:D:125:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:103:LYS:HE2	2:D:179:VAL:HG23	2.03	0.41
2:B:13:LYS:HD2	2:B:85:GLN:HB3	2.02	0.41
1:A:37:ILE:O	1:A:41:MET:HG2	2.21	0.41
1:A:19:PRO:O	1:A:57:ASN:N	2.54	0.41
2:D:168:LEU:HA	2:D:168:LEU:HD23	1.82	0.41
1:A:380:ILE:O	1:A:384:GLY:HA2	2.20	0.41
1:A:540:LYS:HA	1:A:540:LYS:HD3	1.74	0.41
2:B:266:TRP:HD1	2:B:425:LEU:HD13	1.86	0.41
2:B:203:GLU:O	2:B:206:ARG:HB2	2.21	0.41
1:C:58:THR:HG23	1:C:129:ALA:O	2.21	0.41
2:B:170:PRO:HB2	2:B:208:HIS:NE2	2.36	0.41
2:B:358:ARG:NH2	2:B:405:TYR:O	2.53	0.41
2:D:91:GLN:NE2	2:D:92:LEU:HG	2.36	0.41
1:C:330:GLN:NE2	1:C:340:GLN:OE1	2.50	0.41
1:C:187:LEU:HD23	1:C:187:LEU:HA	1.87	0.41
2:D:234:LEU:O	2:D:235:HIS:ND1	2.54	0.41
2:B:114:ALA:H	2:B:214:LEU:HD13	1.85	0.40
4:F:806:DT:H2"	4:F:807:DC:OP1	2.20	0.40
2:D:197:GLN:HG2	2:D:197:GLN:H	1.68	0.40
1:C:5:ILE:HG22	1:C:212:TRP:HD1	1.87	0.40
2:D:96:HIS:ND1	2:D:97:PRO:HD2	2.36	0.40
1:C:47:ILE:HD11	1:C:130:PHE:CE1	2.56	0.40
1:C:108:VAL:HB	1:C:221:HIS:CD2	2.56	0.40
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.56	0.40
6:A:602:3JY:O15	4:P:822:DG:H2'	2.22	0.40
1:A:10:VAL:HG12	1:A:11:LYS:H	1.86	0.40
2:D:278:GLN:N	2:D:302:GLU:OE1	2.55	0.40
1:A:450:THR:HB	1:A:452:LEU:HB2	2.03	0.40
1:C:252:TRP:HE1	1:C:295:LEU:HD11	1.86	0.40
2:B:378:GLU:O	2:B:382:ILE:HD12	2.22	0.40
2:D:34:LEU:O	2:D:38:CYS:HB2	2.22	0.40
1:A:233:GLU:O	1:A:239:TRP:HA	2.22	0.40
1:A:53:GLU:O	1:A:55:PRO:HD3	2.21	0.40
2:B:312:GLU:HB3	2:B:313:PRO:HD2	2.03	0.40
2:D:82:LYS:HE2	8:D:501:SUC:O3	2.21	0.40
1:A:24:TRP:HE3	1:A:25:PRO:HD2	1.85	0.40
1:A:125:ARG:HE	1:A:147:ASN:HA	1.86	0.40
1:A:97:PRO:HG3	1:A:232:TYR:CD1	2.56	0.40
1:C:88:TRP:CD1	2:D:143:ARG:NH1	2.90	0.40
1:A:104:LYS:HE3	1:A:104:LYS:HB2	1.81	0.40
2:B:118:VAL:HG12	2:B:119:PRO:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/556 (100%)	518 (94%)	34 (6%)	1 (0%)	52	84
1	C	552/556 (99%)	526 (95%)	24 (4%)	2 (0%)	39	74
2	B	408/428 (95%)	389 (95%)	19 (5%)	0	100	100
2	D	408/428 (95%)	388 (95%)	20 (5%)	0	100	100
All	All	1921/1968 (98%)	1821 (95%)	97 (5%)	3 (0%)	52	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	C	59	PRO
1	C	4	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	495/497 (100%)	478 (97%)	17 (3%)	44	79
1	C	495/497 (100%)	479 (97%)	16 (3%)	46	81
2	B	373/390 (96%)	363 (97%)	10 (3%)	52	84
2	D	373/390 (96%)	360 (96%)	13 (4%)	43	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1736/1774 (98%)	1680 (97%)	56 (3%)	46 81

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	3	SER
1	A	5	ILE
1	A	8	VAL
1	A	42	GLU
1	A	90	VAL
1	A	107	THR
1	A	109	LEU
1	A	188	TYR
1	A	221	HIS
1	A	237	ASP
1	A	450	THR
1	A	463	ARG
1	A	473	THR
1	A	529	GLU
1	A	547	GLN
1	A	551	LEU
1	C	2	ILE
1	C	3	SER
1	C	5	ILE
1	C	28	GLU
1	C	58	THR
1	C	95	PRO
1	C	101	LYS
1	C	109	LEU
1	C	221	HIS
1	C	270	ILE
1	C	277	ARG
1	C	324	ASP
1	C	338	THR
1	C	471	ASN
1	C	515	SER
1	C	550	LYS
2	B	29	GLU
2	B	64	LYS
2	B	69	THR
2	B	72	ARG

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Mol	Chain	Res	Type
2	B	77	PHE
2	B	139	THR
2	B	156	SER
2	B	195	ILE
2	B	241	VAL
2	B	336	GLN
2	D	11	LYS
2	D	38	CYS
2	D	39	THR
2	D	74	LEU
2	D	75	VAL
2	D	195	ILE
2	D	241	VAL
2	D	274	ILE
2	D	276	VAL
2	D	317	VAL
2	D	322	SER
2	D	425	LEU
2	D	428	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	487	GLN
1	A	507	GLN
1	C	147	ASN
1	C	222	GLN
1	C	373	GLN
1	C	407	GLN
1	C	487	GLN
1	C	507	GLN
2	B	278	GLN
2	B	336	GLN
2	D	151	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	MRG	F	817	1,3,4	20,28,29	3.31	9 (45%)	25,39,42	2.56	9 (36%)
4	MRG	P	817	1,3,4	20,28,29	3.17	9 (45%)	25,39,42	2.46	9 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MRG	F	817	1,3,4	-	1/8/26/27	0/3/3/3
4	MRG	P	817	1,3,4	-	0/8/26/27	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	817	MRG	C2'-C3'	-3.41	1.43	1.52
4	P	817	MRG	C2'-C3'	-3.18	1.44	1.52
4	P	817	MRG	O3'-C3'	-2.48	1.37	1.43
4	F	817	MRG	O4'-C4'	-2.42	1.39	1.45
4	P	817	MRG	O4'-C4'	-2.32	1.39	1.45
4	F	817	MRG	O3'-C3'	-2.22	1.38	1.43
4	P	817	MRG	C2-N3	2.46	1.43	1.34
4	P	817	MRG	C2-N1	2.54	1.43	1.34
4	F	817	MRG	C2-N1	2.80	1.44	1.34
4	F	817	MRG	C2-N3	3.05	1.45	1.34
4	F	817	MRG	C6-C5	3.65	1.48	1.41
4	P	817	MRG	C6-C5	3.69	1.48	1.41
4	F	817	MRG	C6-N1	4.52	1.41	1.33
4	P	817	MRG	C6-N1	4.90	1.42	1.33
4	P	817	MRG	C4-N3	6.19	1.45	1.35
4	F	817	MRG	C4-N3	6.30	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	817	MRG	C2-N2	9.12	1.49	1.34
4	F	817	MRG	C2-N2	9.97	1.50	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	817	MRG	N3-C2-N1	-5.31	118.05	126.22
4	P	817	MRG	N3-C2-N1	-4.85	118.77	126.22
4	P	817	MRG	C5-C6-N1	-3.90	118.26	123.59
4	F	817	MRG	C5-C6-N1	-2.96	119.55	123.59
4	F	817	MRG	O5'-C5'-C4'	2.14	116.95	109.12
4	P	817	MRG	O5'-C5'-C4'	2.29	117.51	109.12
4	P	817	MRG	C21-N2-C2	2.58	128.68	123.80
4	F	817	MRG	C21-N2-C2	2.73	128.96	123.80
4	F	817	MRG	N2-C2-N3	2.91	122.67	117.22
4	P	817	MRG	N2-C2-N3	2.95	122.73	117.22
4	P	817	MRG	C2-N3-C4	3.71	119.55	115.09
4	F	817	MRG	C2-N3-C4	3.98	119.88	115.09
4	P	817	MRG	C22-C21-N2	4.46	123.54	111.46
4	P	817	MRG	O4'-C1'-N9	4.56	115.62	107.72
4	F	817	MRG	C6-N1-C2	4.57	121.95	115.31
4	F	817	MRG	C22-C21-N2	4.61	123.94	111.46
4	P	817	MRG	C6-N1-C2	4.91	122.45	115.31
4	F	817	MRG	O4'-C1'-N9	5.68	117.56	107.72

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	817	MRG	C22-C21-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	817	MRG	1	0
4	P	817	MRG	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	3JY	A	602	5	15,24,25	2.23	2 (13%)	16,36,37	2.82	6 (37%)
8	SUC	B	501	-	24,24,24	0.34	0	36,36,36	0.94	1 (2%)
6	3JY	C	602	5	15,24,25	2.26	2 (13%)	16,36,37	2.49	4 (25%)
7	SO4	C	604	-	4,4,4	0.28	0	6,6,6	0.76	0
8	SUC	D	501	-	24,24,24	0.29	0	36,36,36	0.76	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	3JY	A	602	5	-	0/4/27/29	0/2/2/2
8	SUC	B	501	-	-	0/12/51/51	0/2/2/2
6	3JY	C	602	5	-	0/4/27/29	0/2/2/2
7	SO4	C	604	-	-	0/0/0/0	0/0/0/0
8	SUC	D	501	-	-	0/12/51/51	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	602	3JY	O11-C10	-6.98	1.34	1.44
6	A	602	3JY	O11-C10	-6.83	1.35	1.44
6	A	602	3JY	O1-C2	4.28	1.35	1.24
6	C	602	3JY	O1-C2	4.39	1.35	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	602	3JY	C3-C2-N21	-5.62	118.88	125.14
6	C	602	3JY	C3-C2-N21	-5.15	119.40	125.14
8	B	501	SUC	C6'-C5'-C4'	-2.43	109.34	115.08
8	D	501	SUC	C6'-C5'-C4'	-2.07	110.18	115.08
6	A	602	3JY	C4-C3-C2	2.02	122.66	120.05
6	C	602	3JY	C10-C20-C7	2.27	107.56	102.69
6	C	602	3JY	C20-C7-C8	2.54	106.62	102.62
6	A	602	3JY	C10-C20-C7	2.67	108.42	102.69
6	A	602	3JY	C20-C7-C8	3.42	108.00	102.62
6	A	602	3JY	C8-C9-C10	3.45	109.32	102.59
6	C	602	3JY	C2-N21-C22	6.90	121.21	115.25
6	A	602	3JY	C2-N21-C22	7.26	121.52	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	3JY	4	0
8	B	501	SUC	1	0
6	C	602	3JY	2	0
8	D	501	SUC	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	555/556 (99%)	0.51	61 (10%) 7 4	30, 77, 151, 185	0
1	C	554/556 (99%)	0.66	70 (12%) 5 3	32, 83, 149, 180	0
2	B	412/428 (96%)	0.22	20 (4%) 33 27	28, 60, 101, 126	0
2	D	412/428 (96%)	0.38	33 (8%) 15 10	33, 74, 119, 150	0
3	E	24/27 (88%)	0.91	5 (20%) 1 1	71, 108, 176, 199	0
3	T	24/27 (88%)	0.58	3 (12%) 5 3	66, 99, 176, 190	0
4	F	19/21 (90%)	0.44	2 (10%) 8 5	59, 89, 157, 160	0
4	P	19/21 (90%)	0.04	1 (5%) 30 23	63, 84, 142, 145	0
All	All	2019/2064 (97%)	0.47	195 (9%) 10 6	28, 74, 145, 199	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	LEU	13.5
2	D	4	PRO	11.6
3	T	702	DT	10.2
2	D	214	LEU	9.0
1	A	140	PRO	8.7
1	C	133	PRO	7.3
1	A	73	LYS	7.0
1	A	134	SER	6.6
1	C	132	ILE	6.1
1	A	26	LEU	6.1
1	C	138	GLU	6.1
3	E	702	DT	6.1
1	C	142	ILE	5.9
1	C	293	ILE	5.5
1	C	26	LEU	5.3
1	A	133	PRO	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	61	PHE	5.2
1	A	141	GLY	5.1
1	C	24	TRP	5.1
1	C	130	PHE	5.0
1	C	252	TRP	4.9
1	C	61	PHE	4.9
1	C	58	THR	4.8
1	C	34	LEU	4.8
2	B	4	PRO	4.7
2	B	215	THR	4.7
1	C	136	ASN	4.7
1	C	223	LYS	4.6
1	A	142	ILE	4.6
1	A	62	ALA	4.5
1	C	246	LEU	4.5
1	C	303	LEU	4.5
1	C	28	GLU	4.5
1	C	19	PRO	4.4
1	A	58	THR	4.4
1	A	131	THR	4.4
1	C	134	SER	4.3
2	D	177	ASP	4.3
1	A	293	ILE	4.2
1	A	59	PRO	4.2
1	C	22	LYS	4.1
1	C	144	TYR	4.1
2	D	216	THR	4.1
1	A	136	ASN	4.1
2	D	5	ILE	4.1
1	C	131	THR	4.1
1	C	60	VAL	4.0
1	A	286	THR	4.0
1	C	140	PRO	4.0
1	A	27	THR	4.0
1	C	294	PRO	3.9
1	A	137	ASN	3.9
1	C	287	LYS	3.9
1	A	193	LEU	3.9
1	C	21	VAL	3.8
2	D	90	VAL	3.8
2	B	213	GLY	3.8
1	C	448	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	223	LYS	3.8
1	A	34	LEU	3.7
1	C	25	PRO	3.7
1	C	292	VAL	3.7
1	A	52	PRO	3.7
2	D	89	GLU	3.6
1	C	74	LEU	3.6
2	D	92	LEU	3.6
1	A	289	LEU	3.5
1	C	257	ILE	3.5
2	B	295	LEU	3.5
2	D	231	GLY	3.4
2	B	89	GLU	3.4
2	B	232	TYR	3.4
2	D	212	TRP	3.4
2	B	209	LEU	3.4
1	C	251	SER	3.3
1	A	75	VAL	3.3
1	C	73	LYS	3.3
3	T	725	DG	3.3
1	A	74	LEU	3.3
2	B	88	TRP	3.3
1	A	25	PRO	3.3
1	C	35	VAL	3.2
1	A	56	TYR	3.2
1	C	260	LEU	3.2
2	D	88	TRP	3.1
1	A	19	PRO	3.1
1	C	310	LEU	3.1
1	A	24	TRP	3.1
1	A	50	ILE	3.1
1	A	282	LEU	3.1
1	C	135	ILE	3.1
2	D	168	LEU	3.1
1	A	60	VAL	3.0
1	C	222	GLN	3.0
2	B	217	PRO	2.9
1	A	135	ILE	2.9
1	A	139	THR	2.9
1	A	146	TYR	2.9
1	A	254	VAL	2.9
2	D	360	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	71	TRP	2.9
1	A	144	TYR	2.8
1	A	287	LYS	2.8
1	C	308	GLU	2.8
1	C	20	LYS	2.8
1	C	299	ALA	2.8
1	C	141	GLY	2.8
2	B	250	ASP	2.8
1	A	145	GLN	2.8
1	C	23	GLN	2.8
1	A	127	TYR	2.8
1	C	312	GLU	2.7
2	D	187	LEU	2.7
1	C	221	HIS	2.7
2	D	94	ILE	2.7
2	D	172	LYS	2.7
1	C	139	THR	2.7
1	C	129	ALA	2.7
1	C	67	ASP	2.7
1	C	137	ASN	2.6
2	D	10	VAL	2.7
1	A	132	ILE	2.6
2	D	215	THR	2.6
3	T	703	DG	2.6
2	D	179	VAL	2.6
1	A	285	GLY	2.6
1	A	54	ASN	2.6
1	C	295	LEU	2.6
1	C	271	TYR	2.6
1	A	129	ALA	2.6
1	A	109	LEU	2.6
1	A	77	PHE	2.6
1	A	130	PHE	2.6
1	C	193	LEU	2.6
1	C	198	HIS	2.5
2	B	202	ILE	2.5
2	D	67	ASP	2.5
1	A	39	THR	2.5
1	A	57	ASN	2.5
2	D	358	ARG	2.5
2	D	209	LEU	2.5
2	D	159	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	280	SER	2.5
2	B	301	LEU	2.5
1	C	32	LYS	2.5
1	C	554	ALA	2.5
2	B	428	GLN	2.5
2	D	173	LYS	2.5
3	E	725	DG	2.4
1	C	290	THR	2.4
1	A	222	GLN	2.4
1	A	294	PRO	2.4
1	C	205	LEU	2.4
1	A	288	ALA	2.4
1	C	31	ILE	2.4
1	C	62	ALA	2.4
2	B	231	GLY	2.4
1	A	53	GLU	2.4
1	C	247	PRO	2.4
2	D	95	PRO	2.4
1	C	276	VAL	2.4
3	E	704	DG	2.4
1	C	18	GLY	2.3
2	B	85	GLN	2.3
2	D	93	GLY	2.3
3	E	724	DT	2.3
2	D	178	ILE	2.3
2	D	109	LEU	2.3
2	B	5	ILE	2.3
3	E	703	DG	2.3
2	D	213	GLY	2.3
2	D	7	THR	2.2
2	D	190	GLY	2.2
4	P	803	DC	2.2
4	F	804	DA	2.2
4	F	805	DG	2.2
2	B	252	TRP	2.2
1	C	75	VAL	2.2
1	C	109	LEU	2.2
1	A	30	LYS	2.1
1	C	30	LYS	2.1
1	C	55	PRO	2.1
1	A	234	LEU	2.1
1	A	17	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	204	GLU	2.1
1	A	21	VAL	2.1
1	C	17	ASP	2.0
2	B	86	ASP	2.0
2	D	124	PHE	2.0
1	A	202	ILE	2.0
1	A	283	LEU	2.0
2	D	189	VAL	2.0
1	C	283	LEU	2.0
1	A	49	LYS	2.0
1	A	279	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MRG	F	817	26/27	0.88	0.19	-	93,111,132,135	0
4	MRG	P	817	26/27	0.86	0.17	-	83,98,119,131	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	MG	B	502	1/1	0.83	0.38	7.60	51,51,51,51	0
8	SUC	B	501	23/23	0.86	0.23	1.19	56,72,85,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	SO4	C	604	5/5	0.85	0.28	0.10	74,84,89,104	0
6	3JY	A	602	23/24	0.91	0.20	-0.33	78,89,106,109	0
5	MG	A	603	1/1	0.80	0.17	-0.34	72,72,72,72	0
6	3JY	C	602	23/24	0.93	0.19	-0.38	79,94,106,114	0
5	MG	D	502	1/1	0.96	0.22	-0.82	57,57,57,57	0
5	MG	C	601	1/1	0.79	0.11	-1.11	63,63,63,63	0
8	SUC	D	501	23/23	0.90	0.17	-1.15	66,84,106,106	0
5	MG	C	603	1/1	0.92	0.07	-6.36	113,113,113,113	0
5	MG	A	601	1/1	0.88	0.12	-	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.